Indian J. Phys. **75A** (1), 43-47 (2001)

IJP A

— an international journal

Scattering of a bound polaron in an external laser field

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Abstract : An approach has been proposed to study the scattering cross-sections *e g*, differential (DCS) and momentum transfer (MTCS) of a bound polaron in presence of a coulomb impurity center as well as an external single mode, linearly polarised laser field The main underlying asumptions of the present prescription are (i) the frequency of the laser field (ω_L) is assumed to be much larger than the optical phonon frequency (ω_P), (ii) the electrical component of the laser field intensity (ε_0) is much below the dielectric break down limit, (iii) The interaction of the electron with the phonon field is much stronger than that of the photon field (ε_0), (iv) the electron-phonon coupling parameter (α_P) is taken in the strong coupling region The DCS is always found to be perfectly symmetrical around the scattering angle 90° The variation of the MTCS with respect to α_P, ω_L and the strength of the coulomb impurity (β) have been studied

Keywords : Polarons, laser field, momentum-transfer cross section

PACS Nos. : 71.38 +i

1. Introduction

The problem of a bound polaron (an electron bound by an imperfection in a polar crystal) has drawn attention from both experimental and theoretical physicists [1] since last three decades, particularly in view of its importance in studying the impurity states in polar semiconductors. In fact in such crystals imperfection is a rule rather than an exception. However the previous theoretical studies were mainly limited to the calculation of the ground state energy of the polaron and its transition between low lying states in or without the presence of an external magnetic field.

In the present work, we develop a theoretical approach to study the scattering cross-section of a bound optical polaron from its ground state to a continuum state in presence of a coulomb impurity ion as well as an external laser field. The laser field is chosen to be single mode, linearly polarised, homogeneous electron field represented classically by $\varepsilon(t) = \varepsilon_0 \sin \omega t$, the corresponding vector potential in Coulomb gauge is given by $A(t) = A_0 \cos \omega t$ with $A_0 = c\,\varepsilon_0 / \omega$. Further the electrical component of the laser field is kept much below the dielectric breakdown limit so that all the dielectric parameters of the medium remain unchanged. The frequency of the laser field (ω_L) is assumed to be much larger than the optical phonon frequency (ω_P) so that the interaction of the laser field with the phonon may be neglected as compared to the electron-laser field interaction. The present prescription deals with the strong coupling case for the electron-phonon interaction unlike our previous work [2], where we studied the cross section of a free polaron in presence of a strong laser field with weak electron-phonon interaction (weak coupling case). Since the intensity of the laser field is assumed to be low, the electron-photon interaction is treated as a perturbation in the present work.

As a first step, we use first order time-dependent perturbation theory to calculate the transition probability of the bound polaron from its ground state to a continuum state. We have studied the differential (DCS) as well as total momentum transfer cross sections (MTCS), the latter having direct relevance to the study of transport phenomena (*e.g.* mobility, ac conductivity *etc*) in a dielectric medium in presence of impurity centers.

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2. Theory

The total hamiltonian of the system is the modified version of the Fröhlich hamiltonian [3] and can be written as

$$H = \frac{1}{2m}\left(p - \frac{e}{c}A\right)^2 + \sum_q \hbar\omega_P b_q^+ b_q - \frac{Ze^2}{r\varepsilon_\infty}$$

$$+\sum_q\left[-4i\pi\left(\frac{e^2\hbar}{vq^2\gamma\omega_P}\right)^{\frac{1}{2}}\exp(iq.r)\,b_q + h.c.\right] \quad (1)$$

with

$$\frac{1}{\gamma} = -\frac{\omega_P{}^2}{4\pi}\left(\frac{1}{\varepsilon} - \frac{1}{\varepsilon_\infty}\right),$$

where ε and ε_∞ are the static and the high frequency dielectric constant respectively [1, 3]. A is the vector potential corresponding to the external laser field and $\frac{-Ze^2}{r\varepsilon_\infty}$ denotes the interaction due to coulomb impurity. The dimensionless form of the above hamiltonian is given by

$$H' = \frac{H}{\hbar\omega_P} = -\nabla'^2 - \frac{2\beta}{r'} + \left[A'^2 - 2i(A'.\nabla')\right] + \sum_{q'} b_{q'}^+ b_{q'}$$

$$+\sum_{q'}\left[i\left(\frac{4\pi\alpha p}{v'}\right)^{\frac{1}{2}}\frac{1}{q'}\exp(-iq'.r')\,b_{q'}^+ + h.c.\right], \quad (2)$$

where the dimensionless length $r' = ur$, (u^{-1} being the Fröhlich [3] length unit $\sqrt{\frac{\hbar}{2m\omega P}}$); wave vector $q = qu^{-1}$; volume $v' = vu^3$; coulomb parameter $\beta = \frac{Ze^2u}{2\hbar\omega_P\varepsilon_\infty}$; electron-phonon coupling parameter $\alpha p = \frac{2\pi^2 eu}{\hbar\gamma\omega_P^{\frac{1}{2}}}$ and the dimensionless vector potential $A' = \frac{eA}{cu\hbar}$ (c being the velocity of light). The term $[A'^2 - 2i(A'.\nabla')]$ in eq. (2) can be reduced to (by a canonical transformation [4])

$$A'^2 - 2i(A'.\nabla') = \frac{\partial A'}{\partial t'}.r' = E'.r = \varepsilon_0'.r\sin\omega't' = V_L, \quad (3)$$

where ε_0' is the dimensionless electric field intensity given by $\varepsilon_0' = \frac{eu^{-1}\varepsilon_0}{\hbar\omega_P}$; the dimensionless laser frequency and time are given by $\omega' = \omega_L/\omega_P$, and $t' = \omega_P t$ respectively. Now dropping the primes, the final hamiltonian for the bound optical polaron in presence of a laser field can be written as

$$H = -\nabla^2 - \frac{2\beta}{r} + \sum b_q^+ b_q$$

$$+\sum_q\left[-i\left(\frac{4\pi\alpha_P}{v}\right)^{\frac{1}{2}}\frac{1}{q}\exp(iq.r)b_q + h.c. = H_0 + V_L\right. \quad (4)$$

where V_L is the perturbation (vide eq. (3)).

The unperturbed hamiltonian H_0 satisfies the equation

$$H_0\psi_0 = E_0\psi_0\,. \quad (5)$$

Since in the present work, we deal with the strong coupling case, the unperturbed ground state wave function ψ_0 is chosen to be Pekar-like which is obtained variationally and is given by

$$\psi_0(r,t) = \phi_0(r,t)\,|\chi\rangle, \quad (6)$$

where

$$\phi_0(r,t) = \frac{\beta_c^{\frac{3}{2}}}{\sqrt{\pi}}\exp(-\beta_c r - iE_0 t)$$

with $E_0 = -\beta_c^2 = -(\beta + \frac{5}{16}\alpha_P)^2$ and the normalised phonon wave function (Ref. [1] p 115) is given by

$$|\chi\rangle = \prod |\chi_q \quad (6a)$$

In eq. (6a), all $|\chi_q\rangle$ (q being the phonon momentum) are normalised. The final state wave function of the continuum polaron is chosen as

$$\psi_c(r,t) = \phi_c(r,t)\,|\chi\rangle$$

$$= \frac{1}{\sqrt{v}}\,C\exp(iK_f.r)\,{}_1F_1[i\eta,1,-i(K_f r + K_f.r)]\exp(-iE_f t\,|\chi\rangle \quad (7)$$

with $\eta = \frac{\beta_c}{K_f}$, K_f being the final momentum of the continuum polaron and $C = \exp(\pi\eta)\Gamma(1 - i\eta)$; ${}_1F_1$ is the confluent hypergeometric function. The energy conservation relation for the present system is given by

$$K_f^2 = -\beta_c^2 + \omega. \quad (8)$$

On account of our assumption $\omega_L >> \omega_P$ ($i.e.\ \omega >> 1$), the phonon wave function $|\chi\rangle$ remains unaltered during the time of phonon laser-field interaction. Since the phonon wavefunction $|\chi\rangle$ is normalised, the matrix element for the bound to continuum transition of the polaron is given by

$$T_{if} = <\psi_c|V_L|\psi_0> = \int \phi_c V_L \phi_0\, dr dt. \quad (9)$$

By virtue of eqs. (4), (6) and (7), the eq. (9) can be reduced to

$$T_{if} = -i\sqrt{\frac{\beta_c^3 v}{8\pi^4}}C\int\exp(-iK_f.r)\,{}_1F_1[i\eta,1,i(K_f r + K_f.r)]$$

$$\times(\varepsilon_0.r)\exp(-\beta_c r)dr\int\exp[i(E_f - E_0)t]\sin\omega t\,dt. \quad (10)$$

After performing the t integration in eq. (10) between time $t = 0$ and a later time $t = t_0$ at which the perturbation V_L is turned on and off respectively, we obtain

$$T_{if} = -i\sqrt{\frac{\beta_c^3 \nu}{8\pi^4}} C \int \exp(-i\boldsymbol{K}_f.\boldsymbol{r})_1 F_1\left[i\eta, 1, i(K_f r + \boldsymbol{K}_f.\boldsymbol{r})\right]$$

$$\times (\boldsymbol{\varepsilon}_0.\boldsymbol{r}) \exp(-\beta_c r) dr \quad \frac{\exp\left(i(E_f - E_0 + \omega)\right)t_0 - 1}{E_f - E_0 + \omega}$$

$$\frac{\exp\left(i(E_f - E_0 - \omega)\right)t_0 - 1}{E_f - E_0 - \omega} \tag{11}$$

Since the present study concerns a bound to continuum transition by the absorption of a single photon only, the second term of eq. (11) need be considered [5] because of the fact $E_f > E_0$. The corresponding transition probability per unit time is given by [5]

$$W = (1/t_0) \int \left| T_{if} \right|^2 \rho(k_f)\, dE_{K_f}, \tag{12}$$

where the density of state $\rho(K_f) = (\nu/(2\pi)^3) K_f \sin\theta\, d\theta\, d\phi$. After some mathematical manipulation [5], the expression W in eq. (12) reduces to

$$W = \beta_c^3 C^2 I^2 K_f\ \varepsilon_0^2 \sin\theta\, d\theta\, d\phi \tag{13}$$

where

$$I = \int \exp(i\boldsymbol{K}_f.\boldsymbol{r})_1 F_1(i\eta, 1, K_f r + \boldsymbol{K}_f.\boldsymbol{r})(\boldsymbol{\varepsilon}_0.\boldsymbol{r})$$

$$\times \exp(-\beta_c r)\, dr\,. \tag{14}$$

To calculate the integral I in eq. (14), we now use the following contour integral representation of the confluent hypergeometric function [6]

$$_1F_1(i\eta, 1, z) = \frac{1}{2\pi i} \int_C^{(0^+, 1^+)} dt\, p(\eta, t) \exp(zt) \tag{15}$$

with

$$p(\eta, t) = t^{i\eta - 1} (t-1)^{-i\eta}.$$

Here, C is a closed contour encircling the two points 0 and 1 once anticlockwise. In view of eq. (15), eq. (14) takes the following form

$$I = \frac{1}{2\pi i} \int_C \int \exp(-i\boldsymbol{K}_f'.\boldsymbol{r}) \exp(-\mu r)(\boldsymbol{\varepsilon}_0.\boldsymbol{r}) p(\eta, t)\, dr\, dt \tag{16}$$

where $\mu = \beta_c - iK_f t$; $K_f' = K_f(1-t)$.

To calculate I, the direction of the external field is chosen to be the polar axis. The space integration over $\boldsymbol{r}$ in eq. (16) is now carried out by using standard Fourier transform technique and then the complex t integration is performed analytically with the help of residue calculation method to obtain I in the following closed form :

$$I = \frac{16\pi\mu\varepsilon_0}{} \left(\frac{B}{A-B} \right) \left(A-B \quad K_f \ldots \; B \quad (i\eta - 1) \right.$$

$$\left. - \frac{A}{B}\left(\eta^2 + 5i\eta - 4 + \eta^2 + 3i\eta - 2\right) \right]. \tag{17}$$

In view of eq. (17), the expression for the transition probability W in eq. (13) is obtained in a closed form.

The differential cross section (DCS) which is obtained by dividing the transition probability (W in eq. (13)) by the incident photon flux $\left(\sim \frac{\varepsilon_0^2}{\omega}\right)$ is given by (apart from a scaling factor)

$$\sigma(\theta, \phi) = \beta_c^2 C^2 I^2 K_f^2\, \omega \sin\theta\, d\theta\, d\phi. \tag{18}$$

Finally, the total momentum transfer cross section is given as

$$\sigma_{MTCS} = \int_0^{2\pi} (1 - \cos\theta)\sigma(\theta, \phi) \sin\theta\, d\theta\, d\phi. \tag{19}$$

3. Results and discussion

We have computed the DCS as well as the MTCS for the scattering of a bound polaron in presence of an external laser field of frequency ω_L as well as in the field of a Coulomb impurity centre of strength β.

Figure 1 displays the DCS as a function of the scattering angle θ for some fixed values of β, α_P and ω_l. As is evident from Figure 1 the DCS curves in both the cases show a minimum at an angle $\theta = 90°$ and the curves are found to be perfectly symmetrical about this angle. The curve (1) in Figure 1 refers to a large value of $\alpha_P = 6.3$ while the curve (2) refers to a smaller value, $\alpha_P = 4.8$. The occurrence of this minimum in the DCS in

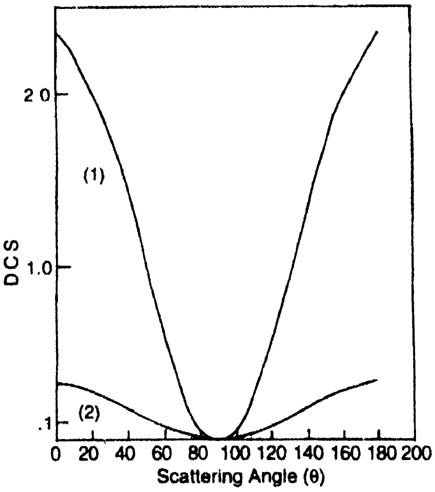

Figure 1. The DCS (in unit of u^{-2}) against the scattering angle θ for $\beta = 1.0$, $\omega \sim 100\omega_L \sim 10^{15}$ (1) for $\alpha_P = 6.3$ and (2) for $\alpha_P = 4.8$

the perpendicular direction of the incident laser field (*i.e.* θ = 90°) may be attributed to the presence of the cosine term ($K_{fz} = K_f \cos\theta$) in the expression of the transiton amplitude (vide eq. (17)). Further, comparing curve (1), (2), it is apparent that the well of the DCS curve becomes shallower with decreasing magnitude of α_P. Similar behaviour of the DCS is noted with respect to the variation of β (not shown in the Figure (1)).

In Figure 2, we have plotted the MTCS *versus* the external laser frequency ω for different combinations of the values of α_P (in the strong coupling region) and β with $\omega\left(=\frac{\omega_L}{\omega_P}\right)$, *e.g.*, curve (1) stands for the set $\beta = 0.0$, $\alpha_P = 4.8$ while curves (2) and (3) represent the sets $\beta = 1.0$ and $\alpha_P = 4.8, 5.7$ respectively. Thus for the fixed value $\beta = 1.0$, the variation of MTCS with respect to α_P can be studied from the comparison of the curves (2) and (3). In contrast, for a fixed value of α_P, comparison of the curves (1) and (2) provides the variation of MTCS with respect of β. It should be noted that all the values of α_P considered in Figure 2 refer to the intermediate and strong coupling region. As may be noted from the Figure, the MTCS curve decreases with increasing ω_L indicating that the bound to continuum transition is suppressed for the high frequency laser field. In fact, for laser frequency $\omega_L \sim 10^{17} - 10^{18}$, the suppression is quite strong *e.g.* the values of MTCS are ~ $10^{-7} - 10^{-8}$ (vide Table 1). As regards the variation of MTCS with respect to β in this Figure, it may be noted that for a fixed value of α_P (= 4.8) the MTCS is higher for $\beta = 1.0$ than for $\beta = 0.0$, which indicates that for the more tightly bound polaron the MTCS is higher since for larger β the final momentum K_f and hence the mobility is smaller (vide eq. (8)).

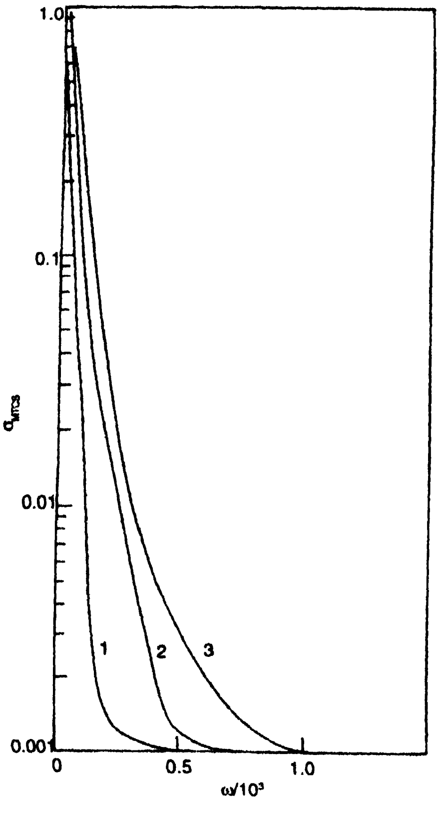

Figure 2. The MTCS (in unit of u^{-2}) *versus* ω (1) for β =0.0, α_P = 4.8; (2) and (3) for β = 1.0 and α_P = 4.8, 5.7 respectively.

In Figure 3 we have plotted the MTCS *versus* the electron-phonon coupling strength α_P for two sets of values of the laser frequency ω_L. As may be noted from the Figure, the MTCS

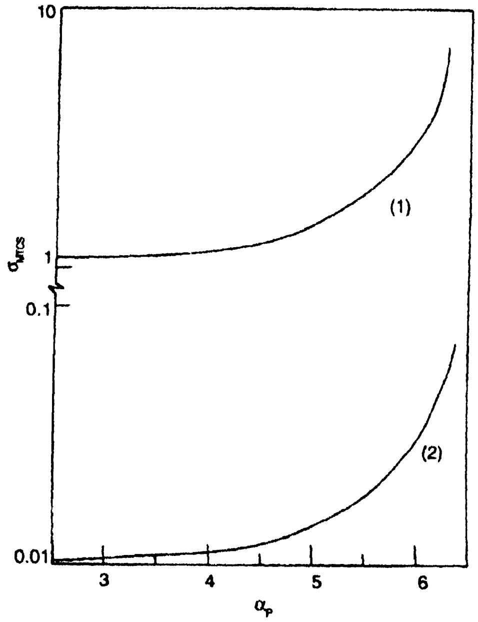

Figure 3. The MTCS *versus* α_P Curve (1) for $\omega_L \sim 10^{16}$ / sec and curve (2) for $\omega_L \sim 10^{17}$ / sec.

Table I. The numerical values of MTCS are quoted in unit of u^{-2} for different values of Fröhlich electron-phonon coupling parameter α_P, coulomb impurity parameter β and laser frequency ω_L (α_P and β are in Fröhlich unit). The MTCS decreases with ω_L and increases with α_P and β.

	$\omega_L = 1.0 \times 10^{15}$		$\omega_L = 1.0 \times 10^{17}$		$\omega_L = 1.0 \times 10^{18}$	
$\beta \rightarrow$ / $\alpha_P \downarrow$	0.0	1.0	0.0	1.0	0.0	1.0
4.8	0.14	0.46	2.0×10^{-6}	1.07×10^{-5}	8.03×10^{-9}	3.66×10^{-8}
5.7	0.209	0.57	3.92×10^{-6}	1.43×10^{-5}	1.31×10^{-8}	4.92×10^{-8}
6.3	–	2.33	–	9.4×10^{-5}	–	3.39×10^{-7}

increases with increasing value of α_p. However this variation is quite slow (almost steady) in the intermediate electron-phonon coupling region ($\alpha_p < 4.5$) while in the strong coupling region ($\alpha_P > 4.5$) the variation is comparatively much rapid indicating that the MTCS is significantly sensitive in the strong coupling region. However, it should be mentioned in this context that the present prescription is particularly suitable for the strong couping case. The comparatively sharp rise of the MTCS in Figure 3 for large α_P (~ 6) may physically be attributed to the fact that the more tightly bound polaron (*i.e.* strong coupling) becomes reluctant to contribute to conductivity. It may further be noticed from Figure 3 that the qualitative behaviour of the MTCS curves (against α_P) remains almost same with respect to the variation of the laser frequency ω_L. Quantitatively, the MTCS is much higher for lower value of ω_L which corroborates the findings in Figure 2.

In Figure 4, we have plotted the MTCS *versus* the coulomb impurity β, keeping other parameters fixed for two different values of α_P, *e.g.* $\alpha_P = 6.3$ (curve (1)) and $\alpha_p = 4.8$ (curve (2)). It is noted from the Figure 3 that for low ω_L the MTCS first increases with β, attains a peak value (depending on the value of α_P) and then again decreases till a cut off, governed by the energy conservation relation (vide eq. (8)) is reached.

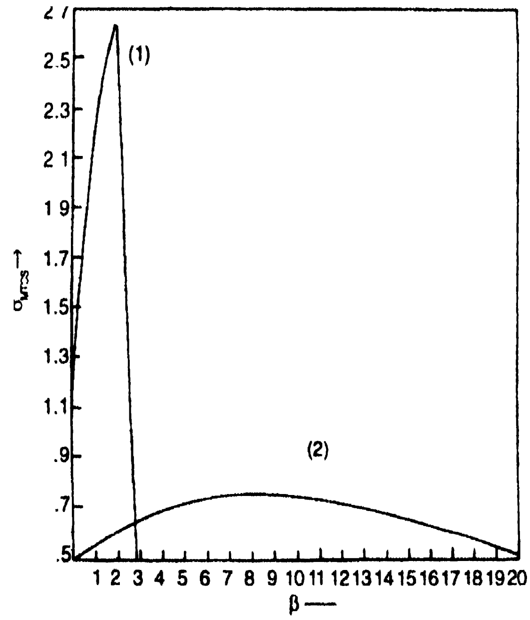

Figure 4. The MTCS *versus* β for ω ~ 100. (1) for α_P = 6.3, and (2) for α_P = 4.2.

In order to have an estimate for the numerical measure of the momentum transfer cross section, we have displayed in Table 1, some MTCS values for different sets of α_P, β and ω_L. It should be mentioned in this context that the values of α_p and ω_p have been taken from Ref. [7].

4. Conclusions

The present theory has been developed mainly for the strong electron-phonon coupling although we have extended it to the intermediate coupling region as well. In this region (strong/intermediate), the scattering cross section increases with the strength of the external laser field in contrast to the weak electron-phonon coupling case [2] where the total cross section was found to be suppressed by the strong laser field. The maximum allowed value of the Coulomb impurity strength β, is restricted by the energy conservation relation (eq (8)) where the ratio $\omega = \omega_L / \omega_P$ plays a significant role. The range of validity for β can be pushed further by increasing the value of ω (*i.e.* by decreasing ω_P or increasing ω_L ; vide eq. (8)).

In the present work, we have calculated the MTCS and DCS for different sets of values of α_P, ω_L and β with electric field intensity ε_0 ~ $10^7 - 10^8$ V/m and $\hbar\omega_L \leq 7.0$ ev which satisfy our approximation that the laser field intensity is within the dielectric breakdown limit and the frequency of laser field does not affect the electron- optical phonon interaction.

Finally, we would like to comment that the present theory neglects the dressing effects of the polaron due to the external laser field which might cause some qualitative change in the dependence of the scattering cross section on the intensity of the external laser field. Calculation including this effect is in progress and will be communicated later.

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